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SURFACE DESIGNS AND PREDICTOR VARIABLE
TRANSFORMATIONS.

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MEASURES OF LACK OF FIT FOR RESPONSE SURFACE DESIGNS
AND PREDICTOR VARIABLE TRANSFORMATIONS[†]

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ABSTRACT

Some first and second order response surface designs are
discussed from the point of view of their ability to detect certain
likely kinds of lack of fit. This leads to consideration of
conditions for representational adequacy of first and second order
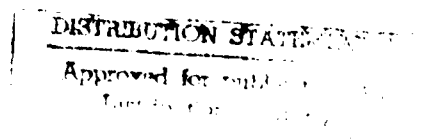models in transformed predictor variables.

MEASURES OF LACK OF FIT FOR RESPONSE SURFACE DESIGNS AND PREDICTOR VARIABLE TRANSFORMATIONS[†]

G. E. P. Box and N. R. Draper

1. INTRODUCTION

Consider a response surface study in which a polynomial of degree d in k predictor variables $\xi_1, \xi_2, \ldots, \xi_k$, is used to represent the expected response $\eta = \eta(\xi_1, \xi_2, \ldots, \xi_k)$. Thus, for $d = 3$, we have a third order model

$$\eta = \beta_0' + \left\{ \sum_{i=1}^{k} \beta_i' \xi_i \right\} + \left\{ \sum_{i=1}^{k} \sum_{j \geq 1}^{k} \beta_i' \xi_i \xi_j \right\}$$
$$+ \left\{ \sum_{i=1}^{k} \sum_{j \geq i}^{k} \sum_{\ell \geq i}^{k} \beta_{ij\ell}' \xi_i \xi_j \xi_\ell \right\}. \qquad (1.1)$$

Denote the observed response by y and suppose that the errors $\varepsilon_u = y_u - \eta_u$ are independently and identically normally distributed with variance σ^2. If, as is usual, we fit models of this kind with predictors coded in "design units"

$$x_i = (\xi_i - \xi_{i0})/S_i, \qquad (1.2)$$

then we can write the model of degree $d = 3$ in the form

$$\eta = \beta_0 + \left\{ \sum_{i=1}^{k} \beta_i x_i \right\} + \left\{ \sum_{i=1}^{k} \sum_{j \geq i}^{k} \beta_{ij} x_i x_j \right\}$$
$$+ \left\{ \sum_{i=1}^{k} \sum_{j \geq i}^{k} \sum_{\ell \geq i}^{k} \beta_{ij\ell} x_i x_j x_k \right\}. \qquad (1.3)$$

Models of orders $d = 1$ and $d = 2$ are obtained by omitting the appropriate bracketed terms in (1.1) and (1.3). To obtain the most parsimonious representation, (usually corresponding to the lowest possible value of d) it may be necessary to transform the response y and/or certain of the predictor variables ξ.

Now whenever we fit a model we face the possibility that some more complex model may be needed. We can try to resolve our doubts by employing a larger design which makes it possible to fit the more complex models, but then similar questions arise concerning <u>that</u> model, and so on. Clearly we cannot guard against all possibilities. A practical compromise is

1. to entertain initially at each stage of the experimental iteration, a model (containing, say, p parameters) which it is hoped will be adequate.

2. to employ an associated design which, with a number of runs only modestly larger than p provides for checks sensitive to particularly feared discrepancies.

3. if such discrepancies occur, to consider first the possibility of their elimination by transformation (or retransformation) of y and/or $\xi_1, \xi_2, \ldots, \xi_k$.

4. because there are situations where a more complex model cannot be avoided, to employ design arrangements which can be conveniently augmented to form larger designs appropriate for fitting and checking the more complex model.

Our object is to consider some appropriate checks and the possible elimination of the associated lack of fit by power transformations of the predictors ξ, for first and second order polynomial models and designs. Transformation of the response y (Bartlett, 1947; Box and Cox, 1964; Kruskal, 1968; Draper and Hunter, 1969) will not be considered here.

2. FIRST ORDER MODELS AND DESIGNS

2.1 Some first order designs with discrepancy checks.

Useful first order response surface designs are the two-level factorials and fractional factorials of resolution three or more which use (respectively) all or some of the 2^k runs $(\pm 1, \pm 1, \ldots, \pm 1)$. As discussed, for example, by Box and Wilson (1951), fractions can be chosen so that checks are associated with the residual degrees of freedom containing feared interactions. Alternatively, or in addition, (see De Baun, 1956), by adding n_0 center points to any such design, a contrast c_2 between the average response $\bar{y}_{co}$ at the center and the average response $\bar{y}_c$ at the factorial points is

$$c_2 = \bar{y}_c - \bar{y}_{co}$$

with   (2.1)

$$E(c_2) = \sum_{i=1}^{k} \beta_{ii}.$$

Thus, in the common situation where the β_{ii} are either of the same sign or are near to zero, c_2 provides an overall check for curvature of second order.

2.2 Can we use a first order model in transformed predictor variables?

When a curvilinear response relationship exists which is monotonic in the predictor variables over the current region of interest, it may be possible

to use a first order model in which power transformations $\xi_1^{\lambda_1}, \xi_2^{\lambda_2}, \ldots, \xi_k^{\lambda_k}$ are applied to the ξ's.

Assume that, <u>at worst</u>, the response may be represented by a second degree polynomial in transformed variables, namely by

$$\eta(\underset{\sim}{\xi},\lambda) = \dot{\beta}_0 + \sum_{i=1}^{k} \dot{\beta}_i \xi_i^{\lambda_i} + \sum_{i=1}^{k} \sum_{j \geq i}^{k} \dot{\beta}_{ij} \xi_i^{\lambda_i} \xi_j^{\lambda_j}. \tag{2.2}$$

Then a first degree polynomial model will be appropriate if the λ_i may be chosen so that $\beta_{ij} = 0$ for all i and j. In Appendix C, we show that this requires that

$$\eta_{ij} = 0, \qquad i \neq j \tag{2.3}$$

$$\eta_{ii} + \delta_i(1-\lambda_i)\eta_i = 0, \qquad i = 1,2,\ldots,k. \tag{2.4}$$

where

$$\eta_i = \left[\frac{\partial \eta}{\partial x_i}\right]_{x_i=0}, \qquad \eta_{ij} = \left[\frac{\partial^2 \eta}{\partial x_i \partial x_j}\right]_{x_i=0} \tag{2.5}$$

and where

$$\delta_i = S_i/\xi_{i0}. \tag{2.6}$$

Now suppose that a second order model of the form of Eq. (1.3) with $d = 2$ has been fitted to the data from an appropriate design. Then we could approximate the derivatives of Eq. (2.5) by

$$\hat{n}_i = b_i/S_i; \qquad \hat{n}_{ij} = b_{ij}/(S_i S_j), \; i \neq j; \qquad \hat{n}_{ii} = 2b_{ii}/S_i^2, \qquad (2.7)$$

Thus (i) the possibility of a first order representation in transformed variables $\xi_i^{\lambda_i}$ is contra-indicated (see Eq. (2.3)) if one or more interaction estimates b_{ij}, $i \neq j$, are significantly different from zero, and (ii) supposing such a transformation to be possible, the appropriate transformation parameters are roughly[*] estimated by

$$\hat{\lambda}_i = 1 + 2b_{ii}/(\delta_i b_i), \qquad i = 1,2,\ldots,k. \qquad (2.8)$$

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[*] More precise estimates can be found by application of standard nonlinear least squares, fitting the model of Eq. (2.2) with $\hat{\beta}_{ij} = 0$ directly to the data.

3. SECOND ORDER MODELS AND DESIGNS

3.1 Some second order designs with discrepancy checks.

A useful class of second order designs (see Box and Wilson, 1951) appropriate for fitting Eq. (1.3) with d = 2 consists of the central composite arrangements in which a "cube", consisting of a two-level factorial with coded points $(\pm1,\pm1,\ldots,\pm1)$ or a fraction of resolution $R \geq 5$ is augmented by an added "star", with axial points at coded distance α, and by n_0 added center points at $(0,0,\ldots,0)$. More generally, both the cube and the star might be replicated. A simple example of a design of this type for k = 2 is defined by the columns headed x_1 and x_2 in Table 1. (We use n_c and n_s for the number of cube and star points and n_{co} and n_{so} for the number of center points associated with them, respectively. Thus $n_0 = n_{co} + n_{so}$. Also shown are some manufactured data whose mode of generation is discussed in Appendix A.

The fitted least squares second degree equation is

$$\hat{y} = 30.59 - 4.22x_1 - 5.91x_2 - 1.66x_1^2 - 1.44x_2^2 - 3.41x_1x_2 \qquad (3.1)$$
$$\pm\,0.25 \quad \pm0.17 \quad\;\; \pm0.17 \quad\;\; \pm0.14 \quad\;\; \pm0.14 \quad\;\; \pm0.24$$

where $\pm$ limits beneath each estimated coefficient indicate estimated standard errors, using the pure error estimate $s_e^2 = 0.457$ to estimate σ^2. An associated analysis of variance table is shown as Table 2.

Table 1. A composite design for k = 2 predictor variables and its associated
estimator columns; $n_c = 8$, $n_{co} = 1$, $n_s = 4$, $n_{so} = 5$, $\alpha = 2$.

I	x_1	x_2	x_1^2	x_2^2	$x_1 x_2$	$x_{111}/1.5$	$x_{222}/1.5$	8CC	Blocks	y
1	-1	-1	1	1	1	1	1	1	-1	37.5
1	-1	-1	1	1	1	1	1	1	-1	38.3
1	1	-1	1	1	-1	-1	1	1	-1	34.7
1	1	-1	1	1	-1	-1	1	1	-1	35.1
1	-1	1	1	1	-1	1	-1	1	-1	27.7
1	-1	1	1	1	-1	1	-1	1	-1	29.2
1	1	1	1	1	1	-1	-1	1	-1	12.2
1	1	1	1	1	1	-1	-1	1	-1	11.4
1	.	.	.	.	.	.		-8	-1	30.1
1	-2	.	4	.	.	-2	.	-1	1	30.2
1	2	.	4	.	.	2	.	-1	1	16.1
1	.	-2	.	4	.	.	-2	-1	1	31.4
1	.	2	.	4	.	.	2	-1	1	16.7
1	.	.	.	.	.	.	.	0.8	1	30.5
1	.	.	.	.	.	.	.	0.8	1	29.9
1	.	.	.	.	.	.	.	0.8	1	29.9
1	.	.	.	.	.	.	.	0.8	1	29.8
1	.	.	.	.	.	.	.	0.8	1	30.2

Table 2. Analysis of variance associated with the second order model and its checks, for the data of Table 1.

Source		df		SS		MS		F
Mean		1		13,938.934				
Blocks		1		7.347		7.347		
First order extra		2		842.907		421.453		
Second order extra		3		188.142		62.714		
Lack	b_{111}	1		7.701		7.701		16.74
of	b_{222}	1	3, 88.923	79.656	29.691	79.656	64.85,	173.17
fit	CC	1		1.567		1.567		3.14
Pure error		8		3.657		0.457		
Total		18		15,069.910				

Before accepting the utility of the fitted equation we would need to be reassured on two questions:

1. Is there evidence from the data of serious lack of fit? If not,

2. Is the change in $\hat{y}$, over the experimental region explored by the design, large enough compared with the standard error of $\hat{y}$ to indicate that the response surface is adequately estimated?

The analysis of variance of Table 2 sheds light on both these questions. Its use to throw light on the second was studied by Box and Wetz (1973); see also Box, Hunter and Hunter (1978, p. 524) and Draper and Smith (1981, pp. 129-133).

Clearly, for this example, it is the marked lack of fit of the second order model that immediately concerns us. In particular, it is natural to be concerned with the possible effects of third order terms. Associated with the design of Table 1 are four possible third order columns namely those formed by creating entries of the form

$$(x_1^3, x_1 x_2^2); \ (x_2^3, x_2 x_1^2). \tag{3.2}$$

These form two sets of two items, as indicated by the parentheses.

Now suppose these third order columns are orthogonalized with respect to the lower order $\underset{\sim}{X}$-vectors. This may be accomplished by regressing them against the first six columns and taking residuals to yield columns x_{111} (from x_1^3). x_{122} (from $x_1 x_2^2$), and so on. Then

$$x_{iii} = -3x_{ijj}, \quad i \neq j \tag{3.3}$$

and the residual vectors are confounded in two sets of two. Furthermore, the columns x_{111} and x_{222} are orthogonal to each other. These vectors, reduced by a convenient factor of 1.5 to show their somewhat remarkable basic form, are given in Table 1.

Consider now the column x_{111} in relation to Figure 1, which shows the projection of the points of the composite design onto the x_1 axis. Denoting the average of the responses at $x_1 = -\alpha, -1, 1, \alpha$ by $\bar{y}_{-\alpha}, \bar{y}_{-1}, \bar{y}_1$, and $\bar{y}_\alpha$, respectively, we see that a contrast c_{31} associated with x_{111} is

$$c_{31} = \frac{1}{36} x'_{111}y = \frac{1}{3}\{\frac{\bar{y}_\alpha - \bar{y}_{-\alpha}}{2\alpha} - \frac{\bar{y}_1 - \bar{y}_{-1}}{2}\} , \tag{3.4}$$

where, for our example, $\alpha = 2$. The expression in the parentheses is an estimate of the difference in slope of the two chords joining points equidistant from the design center. For a quadratic response curve this difference is zero. Thus c_{31} is a natural measure of overall non-quadraticity in the x_1 direction. A corresponding measure in the x_2 direction is, of course, given by $c_{32} = x'_{222}y/36$.

The corresponding sums of squares for these contrasts, given in Table 2, indicate a highly significant lack of fit. Corresponding plots of the residuals against x_1 and against x_2 show a characteristic pattern. A line joining residuals for observations at $x_i = \alpha$ and $x_i = -\alpha$ slopes up, while the tendency of the remaining residuals is down as x_i is increased. We return to discuss these data later.

Figure 1. Projection of design points on the x_i axis for the composite design in two factors given in Table 1. The contrast c_{3i} is an estimate of the difference between the slopes of the two chords.
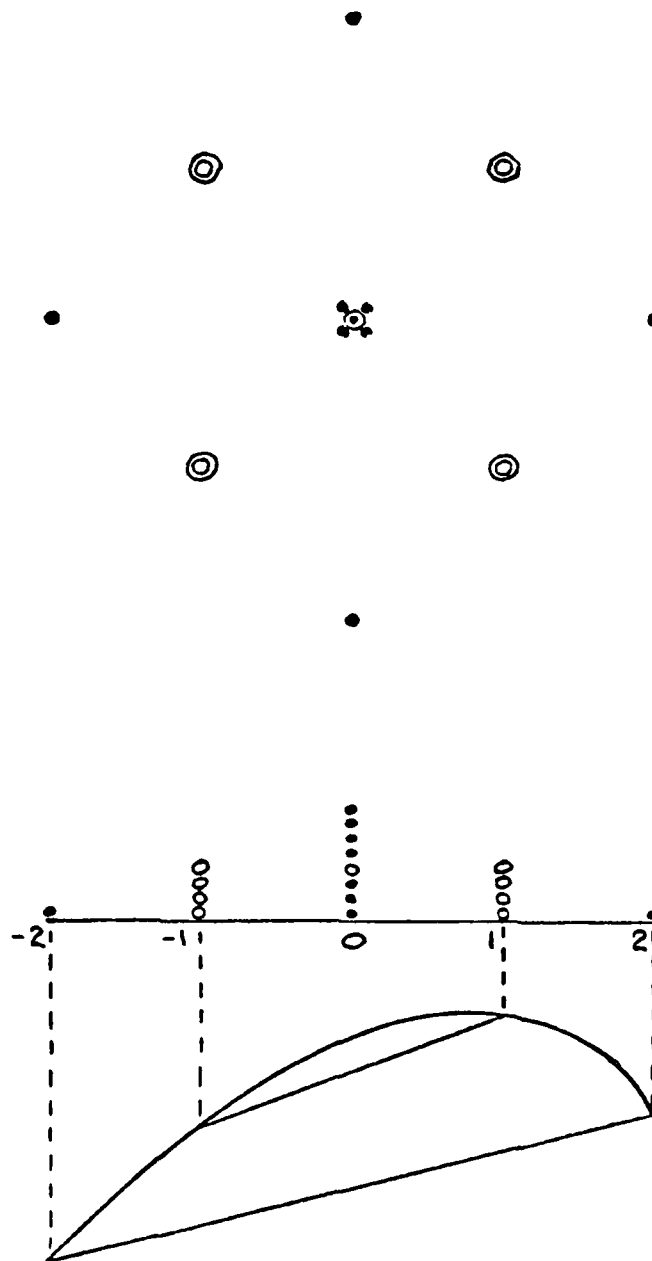
3.2 General formulas.

In general, a composite design contains

(a) A "cube", consisting of a 2^k factorial, or a 2^{k-p} fractional factorial, made up of points of the type $(\pm,\pm 1,\ldots,\pm 1)$, of resolution $R \geq 5$ (Box and Hunter, 1961) replicated $f(\geq 1)$ times. There are thus $n_c = f2^{k-p}$ such points (where p may be zero).

(b) A "star", that is, $2k$ points $(\pm\alpha,0,0,\ldots,0)$, $(0,\pm\alpha,0,\ldots,0),\ldots,$ $(0,0,0,\ldots,\pm\alpha)$ on the predictor variable axes, replicated r times, so that there are $n_s = 2kr$ points in all.

(c) Center points $(0,0,\ldots,0)$, n_0 in number, of which n_{co} are in cube blocks and n_{so} in star blocks.

It is shown in Appendix B that, for any such design, k sets of columns can be isolated with the ith set containing the k columns $x_i x_j^2$, $j = 1,2,\ldots,k$. This ith set is associated with a single vector $\underset{\sim}{x}_{iii}$ which is orthogonal to the $(k+1)(k+2)/2$ columns required for fitting the second degree equation and is also orthogonal to the $(k-1)$ similarly constructed vectors x_{jjj}, $j \neq i$.

The elements of these vectors are such that:

for the cube points, $x_{iii} = \phi x_i$, with $\phi = 2r\alpha^2(1-\alpha^2)/(n_c+2r\alpha^2)$;

for the star points, $x_{iii} = \gamma x_i$, with $\gamma = n_c(\alpha^2-1)/(n_c+2r\alpha^2)$;

for the center points $x_{iii} = 0 = x_i$.

Thus, the k estimates of third order lack of fit, $c_{31}, c_{32},\ldots, c_{3k}$ are

$$c_{3i} = \frac{x'_{iii}y}{x'_{iii}x_{iii}} = \frac{1}{\alpha^2-1} \left\{ \frac{\bar{y}_{\alpha i}-\bar{y}_{-\alpha i}}{2\alpha} - \frac{\bar{y}_{1i}-\bar{y}_{-1i}}{2} \right\} \tag{3.5}$$

with standard deviation

$$\sigma_{c_3} = \frac{1}{\alpha^2-1} \left\{ \frac{1}{n_c} + \frac{1}{2r\alpha^2} \right\}^{1/2} \sigma. \tag{3.6}$$

Also

$$E(c_{3i}) = \beta_{iii} + (1-\alpha^2)^{-1} \sum_{j\ne i}^{k} \beta_{ijj}. \tag{3.7}$$

and the contribution to the lack of fit sum of squares is

$$SS(c_{3i}) = (\alpha^2-1)^2 c_{3i}^2 / \{\frac{1}{n_c} + \frac{1}{2r\alpha^2}\} . \tag{3.8}$$

Note that even if $E(c_{3i}) = 0$, this does not necessarily mean there are no cubic coefficients. A combination of _non-zero_ β_{iii} and β_{ijj} could occur for which $\beta_{iii} + (1-\alpha^2)^{-1} \Sigma\beta_{ijj} = 0$. It is, of course, impossible to guard against every such possibility unless the full cubic model is fitted.

3.3 Can we use a second order model in transformed predictor variables?

In some instances, lack of fit of a second order model, revealed by significant curvature contrasts of the kind just described, might be removed by transformations of some or all of the predictors. A model of this kind contains many fewer parameters than a full third order model and is much easier to analyze and interpret. In order to determine conditions that must be satisfied to make it possible to remove lack of fit in this way, and the part that the curvature contrasts play in this, we suppose that, at worst, the response function may be represented by a third order model in the _transformed_ predictor variables. In Appendix C we show that the conditions that must then apply if all third order coefficients of the transformed $\xi_i^{\lambda_i}$ are to be zero are

$$\eta_{ij\ell} = 0, \quad \text{all } i \neq j \neq \ell = 1,2,\ldots,k; \tag{3.9}$$

$$\eta_{ijj} + \delta_i(1-\lambda_j)\eta_{ij} = 0, \quad i \neq j = 1,2,\ldots,k; \tag{3.10}$$

$$\eta_{iii} + 3\delta_i(1-\lambda_i)\eta_{ii} + \delta_i^2(1-\lambda_i)(1-2\lambda_i)\eta_i = 0, \quad i = 1,2,\ldots,k. \tag{3.11}$$

An important conclusion is thus the following. The possibility of second order representation in the transformed variables is contra-indicated if one (or more) interaction estimates $b_{ij\ell}$ is (are) non-zero.

In practice, the estimation of the transformation (when not contra-indicated) is best done using nonlinear least squares directly on the model of Eq. (2.2); however some interesting light on how the curvature measures c_{3i} relate to these transformations is obtained by considering how Eqs. (3.10) and (3.11) could be used to obtain estimates of the λ_i.

A composite design does not permit all third order terms in Eq. (1.3) to be separately estimated. Suppose, however, that a second order model augmented with only cubic terms

$$\beta_{111}x_1^3 + \beta_{222}x_2^3 + \cdots + \beta_{kkk}x_k^3, \tag{3.12}$$

was fitted. If the response η could be represented by the third order model of Eq. (1.3), the estimates b_i and b_{iii} obtained from the composite design would have expectations

$$E(b_i) = \eta_i - \frac{1}{2}\alpha^2(1-\alpha^2)^{-1} \sum_{j \neq i}^{k} \eta_{ijj} \tag{3.13}$$

$$E(b_{iii}) = \frac{1}{6}\eta_{iii} + \frac{1}{2}(1-\alpha^2)^{-1} \sum_{j \neq i}^{k} \eta_{ijj} \tag{3.14}$$

If now b_i and b_{iii} are used as estimates of the quantities shown as their expectations then, after appropriate substitutions have been made in Eqs. (3.9)-(3.11) we obtain the following k equations for the λ_i. (In these equations, $b_{iii} = c_{3i}$.)

$$b_{iii} + \delta_i(1-\lambda_i)b_{ii} + \frac{1}{6}\delta_i^2(1-\lambda_i)(1-2\lambda_i)b_i$$

$$+ \frac{1}{2}(1-\alpha^2)^{-1}\{1-\frac{1}{6}\alpha^2\delta_i^2(1-2\lambda_i)(1-\lambda_i) \sum_{j \neq i}^{k} \delta_j(1-\lambda_j)b_{ij}\} = 0,$$

$$i = 1,2,\ldots,k. \qquad (3.15)$$

These equations can be solved iteratively. Guessed values for the λ_i are first substituted in the grouping $(1-\lambda_i)(1-2\lambda_i)$ wherever it occurs and the resulting linear equations solved to provide improved estimates for a second iteration, and so on.

For the example data, this procedure converges to the values $\hat{\lambda}_1 = -0.23$, $\hat{\lambda}_2 = -0.93$. These may be compared with the values $\hat{\lambda}_1 = 0.09$, $\hat{\lambda}_2 = -0.82$ provided by nonlinear least squares (these are maximum likelihood estimates under the standard normal error assumptions) and with $\lambda_1 = 0$, $\lambda_2 = -1$, the values used to generate the data; see Appendix A.

An analysis of variance for the transformed data is shown in Table 3 where, as anticipated, no lack of fit appears. (See also Section 3.4 for details.)

Table 3. Analysis of variance for second order model in predictor variables $\ln\xi_1$ and ξ_2^{-1}.

Source	df	SS	MS	
Mean	1	13,938.934		
Blocks	1	7.347	7.347	
First order extra	2	552.713	276.357	535.57
Second order extra	3	565.238	188.413	365.14
Lack $\begin{cases} CC \\ \text{of fit} \; \text{Third order} \end{cases} 3 \begin{cases} 1 \\ 2 \end{cases}$		$2.021 \begin{cases} 1.396 \\ 0.625 \end{cases}$	$0.674 \begin{cases} 1.396 \\ 0.313 \end{cases}$	$1.47 \begin{cases} 3.05 \\ 0.68 \end{cases}$
Pure error	8	3.657	0.457	
Total	18	15,069.910		

3.4. A curvature contrast

Consider the overall curvature measure c_2 of Eq. (2.1) used to check the first order model. When, as in the design of Table 1, center points are available both in the factorial block(s) and in the star block(s) several (two for our example) such measures are available. Consider, specifically, the two block case for a moment. If the average response at the center of the star is $\bar{y}_{so}$ and the average over all the star points is $\bar{y}_{s}$, then the contrast

$$c_2' = \frac{k}{\alpha^2} (\bar{y}_s - \bar{y}_{so})$$

has expectation

$$E(c_2') = \sum_{i=1}^{k} \beta_{ii} \ .$$

Thus the statistic

$$c_2 - c_2' = \bar{y}_c - \bar{y}_{co} - \frac{k}{\alpha^2} (\bar{y}_s - \bar{y}_{so}),$$

which is the difference of the two measures of overall curvature, should be zero if the assumptions made about the model being quadratic are true.

From Figure 1, we see that the curvature measure c_2 associated with the cube (open circles) is contrasted with c_2' associated with the star (block dots). In general the distance from the center of the design to the cube points is $k^{1/2}$ and that for the star points is α. When, as in our example, $k^{1/2}$ and α are different, a significant value of $c_2 - c_2'$ could indicate (for example) a symmetric departure from quadratic fall-off on each side of the maximum, such as we see (for example) in a normal distribution curve.

In general, for two blocks, the standard deviation for $c_2 - c_2'$ is given by

$$\sigma_{c_2 - c_2'} = \{\frac{1}{n_c} + \frac{1}{n_{co}} + \frac{k^2}{\alpha^4} [\frac{1}{2kr} + \frac{1}{n_{so}}]\}^{1/2} \sigma$$

and the associated sum of squares for the analysis of variance table entry of Table 2 is obtained from

$$SS(c_2-c_2') = (c_2-c_2')^2/\{\frac{1}{n_c} + \frac{1}{n_{co}} + \frac{k}{2r\alpha^4} + \frac{k^2}{\alpha^4 n_{so}}\} \; .$$

For our example we find

$$c_2-c_2' = 1.3925 \pm 0.7520$$

with associated sum of squares 1.567 as shown in Table 2. There is clearly no evidence of this sort of lack of fit. When transformed predictors are used, again no lack of fit of this kind is evident, as we see from Table 3.

3.5. Interaction with blocks?

When composite designs are run in blocks, and if we allow the possibility that effects from the predictor variables could interact with blocks, then the various measures of lack of fit would be confounded with block-effect interactions. Although such contingencies must always be borne in mind, it should be remembered that these particular block-effect interactions are no more likely than any others.

SUMMARY

In the traditional analysis of second order response surface designs, a number of degrees of freedom are usually consigned to "lack of fit" and the corresponding sum of squares is used to test for overall lack of fit. Some split-up of lack of fit has been previously discussed (Draper and Herzberg, 1971), but a much more ambitious and detailed division is described here. We show that it is possible to check for cubic lack of fit in the k axial directions and if it exists, not only to check if it is possible to eliminate it by a power transformation in the predictors, but also actually to estimate the powers needed to effect the transformation. The theory is derived in Appendix C, and a worked two-factor example shows how to carry out the calculations.

It is also shown how a certain curvature contrast can be used to check overall quadratic fall-off away from the maximum of a response surface.

Simpler but similar considerations, one degree down, apply to the first order model, and appropriate formulas for these are derived as a special case

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Appendix A. Generation of example data.

Figure Al is taken from the manuscript of a book on response surfaces by G.E.P. Box, N.R. Draper, and J.S. Hunter, in preparation. Figure Al(b) shows a quadratic response function with a simple maximum in variables $(\ln\xi_1, 100\xi_2^{-1})$. This figure is redrawn in the metrics (ξ_1,ξ_2) in Figure Al(a). In the (ξ_1,ξ_2) representation, the doubled cube plus star plus center points design of Table 1 is indicated by the positions of the dots. Response values were calculated at these points, and random error added to give the y-values in Table 1. For these generated data, $\xi_{10} = 2.5$, $\xi_{20} = 12.5$, $S_1 = 0.75$, and $S_2 = 3.75$.
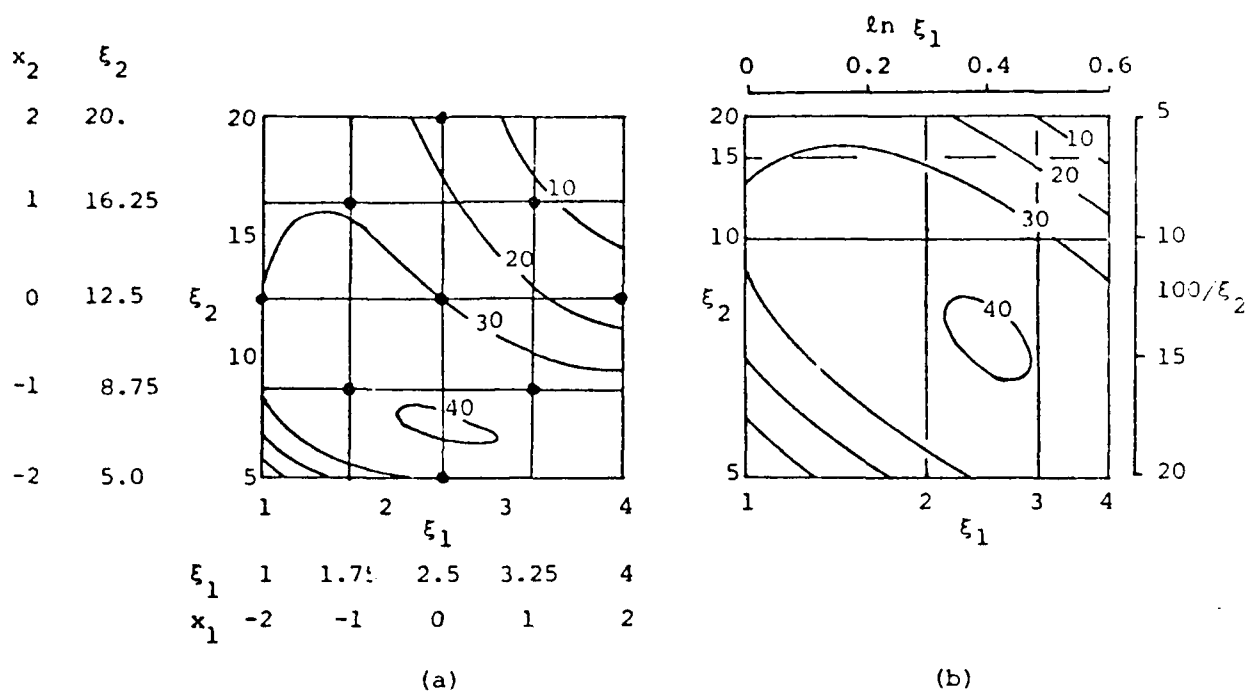
Figure A1. Generation of example data. Surface (a) becomes quadratic, as in (b), when variables $\ln\xi_1$ and ξ_2^{-1} are employed. Data were taken from (a) with added errors.

Appendix B. The third order columns of the $\underset{\sim}{X}$-matrix for a composite design.

We here prove the results summarized in Section 3.2. The full cubic model in k variables $x_1, x_2, \ldots, x_k$ is given by Eq. (3.2). The form of the $\underset{\sim}{X}$ matrix in the regression model $\underset{\sim}{y} = \underset{\sim}{X}\underset{\sim}{\beta} + \varepsilon$ when the design consists of f "cubes" plus r "stars" plus n_o center points is as shown in Table B1. We can denote columns by placing square brackets around the column head; for example $[x_1]$ will denote the x_1 column, and so on. We write $n_c = f2^{k-p}$ for the number of cube points.

All of the cubic columns are orthogonal to all of the other columns with the following exceptions: $[x_i^3]$ is not orthogonal to $[x_i]$, nor to $[x_i x_j^2]$; $[x_i x_j^2]$ is not orthogonal to $[x_i]$, nor to $[x_i^3]$, nor to $[x_i x_\ell^2]$. The first step is to regress the $[x_i^3]$ and $[x_i x_j^2]$ vectors on the $[x_i]$ and take residuals. Because the columns involved are orthogonal to $[x_o]$, no adjustment for means is needed. We denote the "cube portion" of the $[x_i]$ and $[x_i x_j^2]$ vectors by $\underset{\sim}{c}_i$, as indicated in the table. These two sets of residuals are, where the prime denotes transpose,

$$[x_{iii}] = [x_i^3] - \{[x_i]'[x_i^3]/[x_i]'[x_i]\}[x_i] \tag{A1}$$

and

$$[x_{ijj}] = [x_i x_j^2] - \{[x_i]'[x_i x_j^2]/[x_i]'[x_i]\}[x_i] \tag{A2}$$

both of which reduce to multiples $(1-\alpha^2)m$ and m, respectively, where $m = 2r\alpha^2/(n_c + 2r\alpha^2)$, of the same vector. For example,

Table B1. The $\underline{X}$ Matrix For a Cubic Model in k Predictors $x_1, x_2, \ldots, x_k$.

x_0	x_1 x_2 $\ldots$ x_k	x_1^2 x_2^2 $\ldots$ x_k^2	$x_1 x_2$ $\ldots$ $x_{k-1} x_k$	x_1^3 $x_1 x_2^2$ $\ldots$ $x_1 x_k^2$	$x_1 x_2 x_3$ $\ldots$
1	c_1 c_2 $\ldots$ c_k				
1					
$\vdots$	± 1's	1's	± 1's	± 1's	± 1's
$\vdots$	2^{k-p} design		interaction patterns	each column same pattern as in x_1 column	
1					
1	$-\alpha$ $\cdots$ 0	α^2 $\cdots$ 0		$-\alpha^3$	
1	α $\cdots$ 0	α^2 $\cdots$ 0		α^3	
1	$-\alpha$ $\cdots$ 0	α^2 $\cdots$ 0		$-\alpha^3$	
1	α $\cdots$ 0	α^2 $\cdots$ 0	0	α^3	0
$\cdots$	$\cdots$	$\cdots$		$\cdots$	
1	0 $\cdots$ $-\alpha$	0 $\cdots$ α^2		0	
1	0 $\cdots$ α	0 $\cdots$ α^2		0	
1	0 $\cdots$ $-\alpha$	0 $\cdots$ α^2		0	
1	0 $\cdots$ α	0 $\cdots$ α^2		0	
1	0	0	0	0	0
1					
$\cdots$					

(r sets permuted down columns)

$$[x_{111}]' = [c_1', d, -d, d, -d, \ldots, d, -d, 0, 0, \ldots, 0](1-\alpha^2)m, \qquad (A3)$$

where

$$d = n_c/(2r\alpha), \qquad (A4)$$

and where there are r sets of $(d, -d$'s$)$ in the vector. In general, for $[x_{iii}]'$, c_1' will be replaced by c_i' and the position of the $\pm d$'s will correspond to those of the $\mp \alpha$'s in the corresponding $[x_i]'$ vector. Note that, because $c_i'c_j = 0$, $i \neq j$, it is obvious that $[x_{iii}]$ and $[x_{jjj}]$ are orthogonal.

It follows that the k cubic coefficients β_{iii}, β_{ijj} ($j\neq i, j=1,2,\ldots,k$, otherwise) cannot be estimated individually but only in linear combination, and that an appropriate normalized estimating constrast for this is

$$\ell_{iii} = [x_{iii}]'\underset{\sim}{y}/[x_{iii}]'[x_{iii}] \qquad (A5)$$

$$= \{c_i'\underset{\sim}{y}_1 + d(-r\bar{y}_{\alpha i} + r\bar{y}_{-\alpha i})\}/\{n_c(1-\alpha^2)\}$$

where $\underset{\sim}{y}_1$ is the portion of $\underset{\sim}{y}$ corresponding to the cube part of the design, and $\bar{y}_{\alpha i}$, $\bar{y}_{-\alpha i}$ are, respectively the averages of observations taken at the α and $-\alpha$ axial points on the x_i axis. If we similarly denote by $\bar{y}_{1i}$ and $\bar{y}_{-1i}$ the averages of the $n_c/2$ observations in $\underset{\sim}{y}_1$ corresponding to 1 and -1 in c_i, respectively, it follows quickly that $\ell_{iii} = c_{3i}$ where c_{3i} is given in Eq. (3.5). The expected value is

$$E(c_{3i}) = [x_{iii}]'\underset{\sim}{X}'\underset{\sim}{\beta}/[x_{iii}]'[x_{iii}] \qquad (A6)$$

where $\underset{\sim}{X}$ is as in Table B1 and the coefficients of $\underset{\sim}{\beta}$ correspond to the columns in the obvious manner. Because $[x_{iii}]$ is orthogonal to all columns of $\underset{\sim}{X}$ except the $[x_i^3]$ and $[x_i x_j^2]$ columns, Eq. (3.7) emerges almost immediately.

Appendix C. Conditions for efficacy of transformations on the predictor
variables.

Suppose that an experimental design is run in the k coded variables

$$x_i = (\xi_i - \xi_{io})/S_i, \qquad i = 1,2,\ldots,k, \tag{C1}$$

in a situation where the underlying response function can be approximated by a second degree polynomial $F\{(\xi_i^{\lambda_i})\}$ in the transformed __original__ variables $\xi_i^{\lambda_i}$. Thus

$$F(\xi,\lambda) = \beta_0 + \sum_{i=1}^{k} \beta_i \xi_i^{\lambda_i} + \sum_{i=1}^{k} \sum_{j \geq i}^{k} \beta_{ij} \xi_i^{\lambda_i} \xi_j^{\lambda_j} . \tag{C2}$$

Assume all $\lambda_i \neq 0$. (The case when any $\lambda_i = 0$ can be handled as a limiting case using the fact (see, for example, Box and Cox, 1964) that $(\xi^\lambda - 1)/\lambda$ tends to $\ln\lambda$ as λ tends to zero.)

If (C2) is to be a suitable representation, then all third derivatives with respect to the $\xi_i^{\lambda_i}$ must vanish identically. Note that

$$\frac{\partial F}{\partial \xi_i^{\lambda_i}} = \frac{\partial F}{\partial \xi_i} \frac{\partial \xi_i}{\partial \xi_i^{\lambda_i}} = F_i(\xi_i^{1-\lambda_i}/\lambda_i) \tag{C3}$$

say, where $F_i = \partial F/\partial \xi_i$. Moreover, because of Eq. (C1),

$$\eta_i = \frac{\partial F}{\partial x_i} = \frac{\partial F}{\partial \xi_i}\frac{\partial \xi_i}{\partial x_i} = F_i S_i \tag{C4}$$

so that

$$\frac{\partial F}{\partial \xi_i^{\lambda_i}} = \eta_i S_i^{-1}(\xi_i^{1-\lambda_i}/\lambda_i). \tag{C5}$$

The obvious extensions of these results also follow for the higher derivatives which involve terms of the form

$$\eta_{ij} = \frac{\partial^2 F}{\partial x_i \partial x_j} \quad \text{and} \quad \eta_{ij\ell} = \frac{\partial^3 F}{\partial x_i \partial x_j \partial x_\ell}. \tag{C6}$$

If we now carry out the appropriate differentiations, we obtain

$$\frac{\partial F}{\partial \xi_i^{\lambda_i}} = \frac{\xi_i^{1-\lambda_i}}{S_i \lambda_i}\,\eta_i \tag{C7}$$

$$\frac{\partial^2 F}{\partial \xi_i^{\lambda_i}\partial \xi_j^{\lambda_j}} = \frac{\xi_i^{1-\lambda_i}\xi_j^{1-\lambda_j}}{S_i S_j \lambda_i \lambda_j}\,\eta_{ij} \tag{C8}$$

$$\frac{\partial^2 F}{\partial^2(\xi_i^{\lambda_i})} = \frac{\xi_i^{1-2\lambda_i}}{S_i\lambda_i^2}\left[(1-\lambda_i)n_i + \frac{\xi_i}{S_i}n_{ii}\right] \tag{C9}$$

$$\frac{\partial^2 F}{\partial\xi_i^{\lambda_i}\partial^2(\xi_j^{\lambda_j})} = \frac{\xi_i^{1-\lambda_i}\xi_j^{1-2\lambda_j}}{S_iS_j\lambda_i\lambda_j^2}\left[\frac{\xi_j}{S_j}n_{ijj} + (1-\lambda_j)n_{ij}\right] = 0 \tag{C10}$$

$$\frac{\partial^3 F}{\partial^3(\xi_i^{\lambda_i})} = \frac{\xi_i^{1-3\lambda_i}}{S_i\lambda_i^3}\left[\left(\frac{\xi_i}{S_i}\right)^2 n_{iii} + \frac{3\xi_i}{S_i}(1-\lambda_i)n_{ii} + (1-\lambda_i)(1-2\lambda_i)n_i\right] = 0 \tag{C11}$$

$$\frac{\partial^3 F}{\partial\xi_i^{\lambda_i}\partial\xi_j^{\lambda_j}\partial\xi_\ell^{\lambda_\ell}} = \frac{\xi_i^{1-\lambda_i}\xi_j^{1-\lambda_j}\xi_\ell^{1-\lambda_\ell}}{S_iS_jS_\ell\lambda_i\lambda_j\lambda_\ell}n_{ij\ell} = 0. \tag{C12}$$

Eqs. (C10) - (C12) are exact conditions on the λ's. The n_i, n_{ij} and n_{ijk} also involve the λ's, and cannot be specifically evaluated if the λ's are unknown. If <u>estimates</u> of the n_i, n_{ij}, and $n_{ij\ell}$ are substituted, however, Eqs. (C10) - (C12) can be solved to provide estimates of the λ's.

We now assume that the response surface can be approximately represented by a <u>cubic</u> polynomial in the coded predictor variables, namely, by

$$\hat{\eta} = b_0 + b_1 x_1 + \ldots + b_k x_k$$
$$+ b_{11} x_1^2 + \ldots + b_{kk} x_k^2$$
$$+ b_{12} x_1 x_2 + \ldots + b_{k-1,k} x_{k-1} x_k$$
$$+ b_{111} x_1^3 + b_{122} x_1 x_2^2 + \ldots \qquad \text{(C13)}$$
$$+ b_{222} x_2^3 + b_{112} x_1^2 x_2 + \ldots$$
$$+ b_{kkk} x_k^3 + b_{11k} x_1^2 x_k + \ldots$$
$$+ b_{123} x_1 x_2 x_3 + \ldots$$

We can estimate the n_i, n_{ij}, and $n_{ij\ell}$ by the corresponding derivatives of $\hat{\eta}$ evaluated at the center of the design, that is, at $x_i = 0$. In general then,

$$\hat{n}_i = b_i, \qquad \hat{n}_{ii} = 2b_{ii}, \qquad \hat{n}_{iii} = 6b_{iii},$$

$$\text{(C14)}$$

$$\hat{n}_{ij} = b_{ij}, \qquad \hat{n}_{ijj} = 2b_{ijj}, \qquad \hat{n}_{ij\ell} = b_{ij\ell},$$

and we would substitute these in (C10) - (C12), at the same time setting $\xi_i = \xi_{io}$, its value when $x_i = 0$. Note that, from Eq. (C12), we require that $n_{ij\ell} = 0$, which implies that the assumed transformations $\xi_i^{\lambda_i}$ are not suitable representations unless all three-factor interactions are zero. In practice, then, we would want $b_{ij\ell}$ to be small and nonsignificant when $i \neq j \neq \ell$ or else we have a clear indication that the $\xi_i^{\lambda_i}$ will <u>not</u> provide a satisfactory second order representation in (C2). If this aspect is satisfied, however, we now solve the $\frac{1}{2}k(k+1) + k = \frac{1}{2}k(k+3)$ simultaneous equations:

$$\hat{n}_{ijj} + \delta_j(1-\lambda_j)\hat{n}_{ij} = 0, \qquad i \neq j = 1,2,\ldots,k,$$

$$\hat{n}_{iii} + 3\delta_i(1-\lambda_i)\hat{n}_{ii} + \delta_i^2(1-\lambda_i)(1-2\lambda_i)\hat{n}_i = 0, \qquad i = 1,2,\ldots,k \qquad \text{(C15)}$$

where $\delta_i = S_i/\xi_{io}$, and we have divided through Eqs. (C10) and (C11) by factors assumed to be non-zero, namely S_i, ξ_{io}, λ_i, using the $\hat{n}$ values from Eq. (C14).

Composite Designs

An additional complication arises with composite designs. For such designs, we cannot estimate all the third order coefficients individually, as we have explained in Appendix B. This means that, while Eqs. (C15) are still valid, the values in (C14) cannot be used. For a composite design, the column vectors x_i, x_i^3, and $x_i x_j^2$ are linearly dependent via

$$x_i x_j^2 = (-\alpha^2 x_i + x_i^3)/(1-\alpha^2). \qquad \text{(C16)}$$

Thus in the general cubic model, we cannot estimate all $k+k+k(k-1) = k(k+1)$ coefficients in the terms

$$\beta_i x_i + \beta_{iii} x_i^3 + \sum_{j\neq i}^{k} \beta_{ijj} x_i x_j^2 \qquad \text{(C17)}$$

but only the 2k coefficients of

$$\{\beta_i - \frac{\alpha^2}{1-\alpha^2} \sum_{j \neq i}^{k} \beta_{ijj}\}x_i + \{\beta_{iii} + \frac{1}{1-\alpha^2} \sum_{j \neq i}^{k} \beta_{ijj}\}x_i^3. \tag{C18}$$

It follows that, in the model so reduced,

$$b_i \text{ estimates } \eta_i - \frac{\alpha^2}{1-\alpha^2} \frac{1}{2} \sum_{j \neq i}^{k} \eta_{ijj} \tag{C19}$$

while

$$b_{iii} \text{ estimates } \frac{1}{6}\eta_{iii} + \frac{1}{1-\alpha^2} \frac{1}{2} \sum_{j \neq i}^{k} \eta_{ijj}. \tag{C20}$$

(By examining Eqs. (3.7), (C14), and the second portion of Eq. (C18), we infer that $b_{iii} = c_{3i}$.) Alternatively, if the model is fitted using x_i and the "orthogenalized x_i^3", namely $x_{iii} = x_i^3 - \psi x_i$, the terms of the model are

$$\{\beta_i + \psi\beta_{iii} + \theta \sum_{j \neq i}^{k} \beta_{ijj}\}x_i + \{\beta_{iii} + \frac{1}{1-\alpha^2} \sum_{j \neq i}^{k} \beta_{ijj}\}(x_i^3 - \psi x_i) \tag{C21}$$

where

$$\theta = n_c/(n_c+2r\alpha^2), \quad \psi = (n_c+2r\alpha^4)/(n_c+2r\alpha^2) . \tag{C22}$$

In this form, we have that

$$b_i^* \text{ estimates } n_i + \frac{1}{6}\psi n_{iii} + \frac{1}{2}\theta \sum_{j \neq i}^{k} n_{ijj} \tag{C23}$$

and

$$b_{iii}^* \text{ estimates } \frac{1}{6}n_{iii} + \frac{1}{1-\alpha^2}\frac{1}{2}\sum_{j \neq i}^{k} n_{ijj} \tag{C24}$$

where b_i^* is the estimated coefficient of x_i and b_{iii}^* is that for $(x_i^3 - \psi x_i)$. (Note that $b_{iii}^* = b_{iii} = c_{3i}$, but that $b_i^* = b_i + \psi b_{iii}$.) We now describe how this affects the estimation of the λ_i. From Eqs. (C10) and (C11), and setting $\xi_i = \xi_{io}$ we have

$$n_{ijj} + \delta_j(1-\lambda_j)n_{ij} = 0 \tag{C25}$$

and

$$n_{iii} + 3\delta_i(1-\lambda_i)n_{ii} + \delta_i^2(1-\lambda_i)(1-2\lambda_i)n_i = 0 \tag{C26}$$

We now combine $\frac{i}{6}$ times (C26) with $\{\frac{1}{2(1-\alpha^2)} - \frac{\alpha^2}{12(1-\alpha^2)}\delta_i^2(1-2\lambda_i)(1-\lambda_i)\}$ times (C25) summed over $j \neq i$ to give, for $i = 1,2,\ldots,k$,

$$\{\frac{1}{6}n_{iii} + \frac{1}{2}\frac{1}{1-\alpha^2}\sum_{j\neq i}^{k}n_{ijj}\}$$

$$+ \frac{1}{2}\delta_i(1-\lambda_i)n_{ii}$$

$$+ \frac{1}{6}\delta_i^2(1-\lambda_i)(1-2\lambda_i)\{n_i - \frac{\alpha^2}{1-\alpha^2}\frac{1}{2}\sum_{j\neq i}^{k}n_{ijj}\} \qquad (C27)$$

$$+ \frac{1}{2}\frac{1}{1-\alpha^2}\{1-\frac{1}{6}\alpha^2\delta_i^2(1-2\lambda_i)(1-\lambda_i)\}\sum_{j\neq i}^{k}\delta_j(1-\lambda_j)\,n_{ij} = 0.$$

Thus, if the third order model is fitted in terms of x_i and x_i^3 (rather than x_i and $(x_i^3 - \psi x_i)$ as described above) we can substitute appropriate estimates to give the k simultaneous equations for $i = 1,2,\ldots,k$.

$$b_{iii} + \delta_i(1-\lambda_i)b_{ii} + \frac{1}{6}\delta_i^2(1-\lambda_i)(1-2\lambda_i)b_i$$

$$+ \frac{1}{2}\frac{1}{1-\alpha^2}\{1-\frac{1}{6}\alpha^2\delta_i^2(1-2\lambda_i)(1-\lambda_i)\}\sum_{j\neq i}^{k}\delta_j(1-\lambda_j)b_{ij} = 0$$

$$\qquad (C28)$$

which can be solved for $\lambda_1,\lambda_2,\ldots,\lambda_k$. These awkward equations can be difficult to solve unless some care is applied. We suggest an iterative procedure in which rough estimates of λ_i are used in the grouping $Q_i \equiv (1-\lambda_i)(1-2\lambda_i)$ which occurs in two positions in Eq. (C28). The resulting linear equations in $\theta_i = 1-\lambda_i$ are straightforward to solve, and the results are used in the grouping $(1-\lambda_i)(1-2\lambda_i)$ for a second iteration and so on, until convergence is

achieved. To aid convergence, each new iteration can be started from the
midpoint of the old and new values, if desired.

Alternative Cubic Case

If the cubic is fitted with estimated terms $b_i^* x_i + b_{iii}^* (x_i^3 - \psi x_i)$ as
described above, we obtain b_i and b_{iii} from

$$b_i = b_i^* - \psi b_{iii}^* \quad \text{and} \quad b_{iii} = b_{iii}^*. \tag{C29}$$

Related Work

The expression in (C20) can be alternatively written in the form

$$\beta_{iii} + (1-\alpha^2)^{-1} \Sigma \beta_{iij}.$$

Draper and Herzberg (1971, p. 236) show that the sum of squares of these
quantities for $i = 1, 2, \ldots, k$ occurs in the expected value of a general measure
of lack of fit L_1. Thus, the c_{3i} contrasts essentially provide a split-up of
L_1 which permits a more detailed and sensitive analysis. The remaining degrees
of freedom pertaining to L_1 can be attributed to other contrasts as already
described.

The First Degree Case

We return to the beginning of this Appendix to examine the simpler case
when the underlying response surface can be approximated by a first degree
polynomial in the transformed variables $\xi_i^{\lambda_i}$. In such a case

1. All $\beta'_{ij} = 0$, in (C2).

2. All second derivatives with respect to $\xi_i^{\lambda_i}$ must vanish identically.

This condition provides, from Eqs. (C8) and (C9), the equations (2.3) and (2.4).

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Some first and second order response surface designs are discussed from the point of view of their ability to detect certain likely kinds of lack of fit. This leads to consideration of conditions for representational adequacy of first and second order models in transformed predictor variables.

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